Quantification and Simulation of Particle Kinematics and Local Strains in Granular Materials Using X-ray Tomography Imaging and Discrete Element Method

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ABSTRACT

Micro features have significant effects on the macro behavior of granular materials. However, Three-dimension (3D) quantitative measurements of micro features are rare in literature due to the limitations of conventional techniques in obtaining micro quantities such as micro displacements and local strains. This paper presents a new method to quantify the particle kinematics and local strains for a confined compression test using X-ray Computed Tomography (XCT), and a comparison between the experimental measurements and the simulated results using the Discrete Element Method (DEM). The method can identify and recognize 3D individual particles automatically, which is essential for quantification of particle kinematics and local strains. 3D DEM simulations of the confined compression test were performed using spherical particles and irregular particles respectively. The simulated global deformations and particle translations based on irregular particles showed better agreement with the experimental measurements than those based on spherical particles. The simulated movements of spherical particles are more erratic and the material composed of spherical particles has larger vertical contraction and radial dilation.

KEY WORDS

Granular Material, Three-Dimensional Measurement, Micro-Macro, Particle Motion, Local Strain, Local Deformation, Irregular Particles, DEM Simulation, X-ray Tomography, Compression Test
NOTATION

\[ DISP \] Magnitude of particle translational displacement
\[ \Delta H \] Space between two adjacent slices
\[ SI \] Similarity index of particle cross sections
\[ SI_p \] Similarity index of particle
\[ V \] Volume
\[ V_f \] Volumetric fraction
\[ u \] Particle displacement in x direction
\[ v \] Particle displacement in y direction
\[ w \] Particle displacement in z direction
\[ \varepsilon \] Global Strain
\[ \varepsilon' \] Local strain

INTRODUCTION

In the last three decades, research on the behavior of granular materials has been focused on shear banding (Rice 1980; Bardet 1990, 1991; Iwashita 1998), liquefaction (Darve 1996; Lade 2002) and dilatation (Evesque 1993; Oda 1997). It has been found that micro features have significant effect on the behavior of granular materials, but how micro quantities are related to macro properties is not well known yet (Oda and Iwashita 1999). The main reason is that micro features of granular materials are difficult to quantify due to the limitation of conventional techniques for obtaining certain micro quantities such as micro displacements, fabric quantities and micro strains. Recent quantification of the particle motions and strains is usually based on 2D measurements and does not have the capability to measure the out-of-plane particle motions.
(DeJong and Frost 2002; Wang et al. 1999). Few quantitative measurements of the micro
deformation are available in 3D scheme. One of the challenges for 3D micro feature
quantification is to identify individual particles. The existing method for particle identification
requires human judgment (Wang 2004). Thus there is a need for an enhanced method that can
increase the efficiency of experimental data processing for automatically identifying and
recognizing 3D individual particles.

The discrete element method (DEM) was introduced by Cundall (1971) for the analysis of
rock-mechanics problems. It has been increasingly applied to the study of the behavior of
DEM was originally developed to investigate the validity of various continuum models, it has
become a promising tool to study the behavior of granular materials by taking into account the
interactions among constituents and providing better understanding of the granular system at
particle level (Oda 1999). However, DEM approaches generally use spheres, ellipsoids or
computer generated particle configurations to represent real irregular particles in the simulation
(Cundall 1971; Cundall and Strack 1979; Thornton 1998; Rothenburg et al, 1989; Mirghasemi
2002). How well these simulations depict the properties of materials in real condition is not well
established. Since the most significant difference between a real granular system and a simplified
material system is particle shape, it is necessary to investigate the effect of particle shape on the
simulation results. Attempts have been made to simulate elliptical systems in both 2D
(Rothenburg 1992) and 3D (Lin and Ng 1997). More complicated particle shapes can be
modeled using superquadrics (Williams 1991) or bonding a number of spheres together (Walton
and Braun 1993). There has been research in reference to the effect of particle shape on
simulation results, but it could only predict the behavior of granular materials qualitatively
(Jensen et al 2001). How to quantitatively simulate the micro-mechanic properties of real
granular materials, such as micro displacement and micro-strain field of irregular particle system, is still a problem. Even if the simulated micro quantities are obtained, much work needs to be done in evaluating the accuracy of the simulated results. This study provides an insight to the simulated results and the experimental validations based on the actual microstructure of materials.

OBJECTIVES

This study has a number of objectives related to the study of particle kinematics and local strains in real granular materials. The first objective is to develop a valid experimental methodology to quantify global strains, global deformations, local strains and local displacements of granular materials. The second objective is to simulate the global and local strains, particle motions using DEM in which irregular particle shape is taken into account. The third objective is to compare experimental analysis results with those from DEM simulations and evaluate the contribution of irregular particle shape to the micro-macro behavior of granular materials. For the first objective, the first step is to develop a method to automatically identify individual particles with irregular shape, and then calculate particle kinematics and local strains in 3D scheme by comparing the mass center coordinates and orientations of particles before and after the test. For the second and third objectives, simulations using real irregularly-shaped particles and ideal spherical particles were performed and compared.

BACKGROUND

X-ray Tomography Imaging

X-ray computerized tomography (XCT) imaging is a technique to acquire a stack of sectional images non-destructively. Compared to conventional destructive methods, which can be applied only on the surface of a specimen, XCT has the advantage of acquiring the internal
microstructure in a non-destructive manner with high accuracy (Wang, 1999). Compared to other non-destructive techniques such as Magnetic Resonance Imaging (MRI, Lizak et al, 1991) and Laser-Aided Tomography (Konagai et al. 1992), XCT imaging has the advantages of powerful penetrating ability and high sensitivity to material density. Furthermore it needs no special treatment of the specimen as MRI does. The high resolution of industrial XCT is up to 0.01 mm, which provides the required resolution to measure the details at individual particle level. Thus XCT has been more widely used to obtain the microstructure of a material and to investigate the microscopic feature within the material. The herein developed analytical procedure of x-ray images can also be used for images acquired by other methods such as MRI.

EXPERIMENTAL QUANTIFICATIONS

Materials and experimental setup

A compression test with lateral sponge confinement on coarse aggregates was conducted to induce desired particle movements and structural deformations. Limestone aggregates passing 1/2” sieve but retained on 3/8” sieve were used. The aggregates were put into a transparent cylindrical container (100mm high, 103mm diameter), which was specially designed for the convenience of x-ray scanning. A piece of sponge was placed along the inside wall of the container to allow some lateral displacements of individual aggregates to be discernable. Using X-ray tomography imaging, 2D images of the specimen cross sections were acquired slice by slice from bottom to top of the specimen. Then an axial load was applied on the top of the aggregates. The physical properties of the material, load and specimen are presented in Table1. The specimen was scanned by X-ray again and images of the deformed microstructure were acquired after the test. Based on the images acquired before and after the compression test,
material microstructure, particle kinematics and local strains can be obtained using the following methodology.

**Particle Identification**

Particle identification is essential for the 3D representation of microstructure. After gray images were acquired by XCT, the software named Image Pro Plus was used to process the gray images and obtain the digitized geometric properties of individual particle cross sections such as the mass center coordinates and area. Each particle cross section (i) in each slice (z) was denoted as PC(i,z). The next step was to identify which particle cross sections in sectional slices belong to a specific particle, namely a 3D reconstruction procedure. A similarity index (SI) method to identify individual particles from granular media was presented elsewhere (Wang et al. 2004). Further research has shown that some enhancement could be made to improve the efficiency of identification. Recognizing that the particle identification is very sensitive to mass center coordinates, a modified similarity index method was employed in this study. Two particle cross sections in two adjacent slices were considered to belong to the same particle, if a minimum SI \((SI_{\text{min}})\) was obtained using the following equation:

\[
SI(i, z)_{\text{min}} = \min\left | x_{i,z} - x_{j,z+1} \right | + \left | y_{i,z} - y_{j,z+1} \right |
\]

\[i = 1, 2, \ldots n\]

\[j = 1, 2, \ldots m\]

Where \(n\) and \(m\) represent the number of particle cross sections in adjacent slices \(z\) and \(z+1\); \(x, y\) are mass center coordinates of the \(i\)th particle in \(z\)th slice or \(j\)th particle in \((z+1)\)th slice. Using this equation, each particle cross section in slice \(z\) could find its corresponding cross section in slice \(z+1\).

There are three possibilities that could confuse the judgment in individual particle identification:
1) A new particle emerges in the (z+1)th slice. In this case, no corresponding particle cross section could be found in the zth slice. (Figure 1) Then a new code is assigned to this new particle.

2) Existing particle cross sections disappear in the next slice (z+1). In this case, n<m. One particle cross section in slice (z+1) would correspond to two or more particle cross sections in slice z with SI_{min}. Then the pair cross sections PC(i,z) and PC(j,z+1) with smallest SI_{min} are considered to belong to the same particle. Any other particle cross sections in slice z corresponding to the particle cross section PC(j,z+1) are those that disappear in slice (z+1) (Figure 2).

3) An existing particle disappears in the (z+1)th slice while a new particle emerges in that slice almost at the same location, having similar mass center coordinates (Figure 3). Then the trend of the area change of the particle cross-section at slice z-1, z, z+1, z+2 is traced. In this case, the trend must satisfy the relationship \( Area_{z-1,j} > Area_{z,j} \) & \( Area_{z+1,j} < Area_{z+2,j} \), otherwise, those cross sections are still considered to belong to the same particle.

The whole procedure is presented as a flow chart in Figure 4. Based on the above method, a FORTRAN program was developed to automatically identify individual particles from the measured data. Each identified particle was assigned a code k (k=1, 2, 3...). With this code, the corresponding mass center and area of cross section i for particle k in image slice z could be found. Table 2 presents the calculated SI_{min} between pairs of particle cross sections in slices No.70 and No.71. Table 3 presents the geometrical information for the identified cross-sections of particle No.50 in sectional slices. With these data, the microstructure of specimen could be represented, which is essential for experimental quantification and numerical simulation.

**Quantification of Particle Translational Kinematics in 3D**
After being sustained under a compression force, the microstructure of the granular material would change accordingly. If the change of locations and orientations of the individual particles were recorded, the kinematics of the particles can then be calculated based on mathematical relationships. For the confined compression test, the particle displacements were relatively small compared to the size of the aggregates, and the coordinates of the mass center of individual particles changed little in radial direction. Judgment can still be made based on the SI method for individual particles. The particle similarity index ($SI_p$) is defined as follows:

$$SI_p = |x_b - x_a| + |y_b - y_a| + |z_b - (z_a + \frac{\Delta h}{h} \cdot z_a)|$$

Where $x_b,y_b,z_b$ = mass center coordinates of individual particles before test

$x_a,y_a,z_a$ = mass center coordinates of individual particles after test

$\Delta h$ = vertical global deformation of the specimen

$h$ = height of the specimen

The pair of particles giving the smallest $SI_p$ is considered to be the same particle. If two or more particles after test are paired to the same original particle, then their volumes are compared and the one whose volume is closest to that original particle is recognized. The same procedure of finding another original particle giving the smallest $SI_p$ is followed for the remaining particles. This process is repeated until all the particles after test are recognized. The detailed calculation flow chart is presented in Figure 5.

The magnitude of particle translations can then be calculated as

$$DISP_k = \sqrt{u^2 + v^2 + w^2}$$

Where $u = x^a - x^b$; $v = y^a - y^b$; $w = z^a - z^b$, and the superscript “a” denotes after the deformation and “b” denotes before the deformation.

Computation of Micro Motions and Local Strains in 3D
A two-dimensional (2D) experimental method was developed by Wang et al (1999) to measure the particle motions by comparing images of the cross sections of a specimen acquired before and after the test. The 2D method can be extended to 3D by including the motions in z direction. Local strains can be computed following the Finite Element Method (FEM). Suppose four adjacent particles form a tetrahedron (4 nodes, i.e. Figure 6). The local strain components can be computed by treating the four mass centers as the four nodes of the tetrahedron element, using the following equations:

\[ \varepsilon_x = \frac{\partial u}{\partial x} = a_1; \]  
\[ \varepsilon_y = \frac{\partial v}{\partial y} = b_2; \]  
\[ \varepsilon_z = \frac{\partial w}{\partial z} = c_3 \]

\[ \varepsilon_{xy} = \frac{1}{2} \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) = \frac{b_1 + a_2}{2}; \]

\[ \varepsilon_{xz} = \frac{1}{2} \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) = \frac{a_3 + c_1}{2}; \]

\[ \varepsilon_{yz} = \frac{1}{2} \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) = \frac{b_3 + c_2}{2} \]  

\[ a_0, a_1, a_2; b_0, b_1, b_2; c_0, c_1, c_2 \] can be obtained using the following equations:

\[
\begin{bmatrix}
1, x_i, y_i, z_i \\
1, x_j, y_j, z_j \\
1, x_k, y_k, z_k \\
1, x_l, y_l, z_l
\end{bmatrix}
\begin{bmatrix}
a_0 \\
a_1 \\
a_2 \\
a_3
\end{bmatrix}
= 
\begin{bmatrix}
\begin{bmatrix}u_i\end{bmatrix} \\
\begin{bmatrix}u_j\end{bmatrix} \\
\begin{bmatrix}u_k\end{bmatrix} \\
\begin{bmatrix}u_l\end{bmatrix}
\end{bmatrix},
\]
The global strains of the entire specimen are measured by:

\[ \varepsilon_1 = \frac{\Delta h}{h} \quad (6.a) \]

\[ \varepsilon_2 = \varepsilon_3 = \frac{\Delta r}{r} \quad (6.b) \]

\[ \varepsilon_{12} = \varepsilon_{13} = \frac{\varepsilon_1 - \varepsilon_2}{2} \quad (6.c) \]

Where \( \Delta h, h \) = vertical displacement and the height of the specimen;

\( \Delta r, r \) = displacement in the radial direction and the radius of the specimen.

The global volumetric strain is defined as:

\[ \varepsilon_V = \varepsilon_1 + \varepsilon_2 + \varepsilon_3 = \varepsilon_1 + 2\varepsilon_2 \quad (7) \]

The global volumetric strain can also be calculated from the sum of weighted local volumetric strain by the following equation:

\[ \varepsilon_V^I = \sum V_{i\beta} \varepsilon_{V\beta}^I = \sum V_{i\beta} (\varepsilon_{1\beta}^I + \varepsilon_{2\beta}^I + \varepsilon_{3\beta}^I) \quad (8) \]

where \( \varepsilon_V^I = \) global volumetric strain calculated from local volume strain

\( V_{i\beta} = \) volumetric fraction of each local volume to the total volume

\( \varepsilon_{i\beta}^I = \) local strain in tetrahedron \( i \).
Comparing the global volumetric strain calculated by direct measurements and that calculated by weighted local volumetric strains, the local strain quantification methodology can be evaluated.

**Analysis of Experimental Results**

The measured mass center coordinates and the displacements for 10 individual particles are presented in Table 4. The local macro strains in each tetrahedron, calculated by equation (4) are presented in Table 5. The local strains \( \epsilon_x \) at height \( z=45\sim55 \text{ mm} \) were projected on x-y plane, contours of which are presented in Figure 7. Strain \( \epsilon_x \) showed a tendency of dilation from center to edge but there still exists a small contraction at the edge due to the boundary confinement. Figure 8 presents the contours of strain \( \epsilon_z \) at \( y=45\sim55 \text{ mm} \) projected on x-z plane. Most of the regions show a tendency of strain contraction and most of the contraction occurs at the top of the specimen. Strain dilation also exists in the center region.

In Figure 8, a vertical line was drawn at \( x=50\text{mm} \) from top to bottom, and the values of local strain \( \epsilon_z \) at the vertical line were read every 10 mm (i.e. \( dz=10 \text{ mm} \)). Thus the total deformation of \( z \) direction can be calculated as \( \Delta z = \sum \epsilon_z dz = -9.2 \text{mm} \), which is very close to the measured vertical deformation, 9.8 mm. The global volumetric strain calculated by equation (7) is 0.047 and that calculated by equation (8) is 0.052, which are also close to each other. Thus the validations of the methods to quantify the local strains are acceptable.

**PFC\(^{3D}\) and DEM SIMULATION**

In order to study the particle shape effect on the micro-macro behavior of granular materials, Particle Flow Code in Three-Dimensions (PFC\(^{3D}\)) was used to conduct DEM simulation on irregular particles and on spherical particles respectively. The actual
microstructure used in confined compression test was incorporated into the simulation. Irregular particles were represented by clusters of balls. Each cluster behaves as a rigid particle with deformable boundaries in PFC\(^3\text{D}\) (Itasca 1999). A burn algorithm was applied to reduce the required number of balls so that the calculation efficiency can be greatly improved (Fu and Wang 2005). The virtual specimen composed of 173 particles in PFC\(^3\text{D}\) is illustrated in Figure 9. The spherical particles were generated using the particle mass centers and volumes same as those of irregular particles. The virtual specimen using spherical particles is depicted in Figure 10.

In the simulation, the particles were virtually stacked in a cylindrical container and a rigid load plate was placed on the top of the aggregates. The load plate was made from hundreds of strongly bonded balls that would break apart during the simulation. An axial force was applied directly on the load plate. The physical properties of particles, boundary and compact force were assigned similar to those in the confined compression test.

**Simulation Results and Comparison to Experimental Measurements**

The simulated coordination number based on irregular particles and spheres were calculated and compared to the experimental measurements (Table 6). The change of coordination number based on spheres was bigger than that based on the real structure. The change in porosity by experimental measurement was 2.4% while that by simulation was 2.3% based on irregular particles and 2.7% based on spheres. These results are compatible with the trend that materials composed of rounded particles have better workability to be compacted than those composed of irregularly-shaped particles (Roberts et al, 1996).

The particle translational movements by simulations and by actual experiment are illustrated in Figure11~Figure13. Most of the simulated irregular particle movements occurring in the vertical direction and at the lower part of the sample were very small, which was similar to
the trend of experimental observations. However, simulated movements of spherical particle are more erratic. The simulated magnitudes of particle translations versus experimental measurements were plotted in Figure14 and Figure 15. Most of the points based on irregular particles are located around the 45° line while those based on spherical particles are much scattered. This means the simulated irregular particle translations have better agreement with experimental observations than those based on spherical particles. The data points based on irregular particles still had some discrepancy from the experimental results. This may be caused due to several reasons. First of all, using clusters of balls to represent irregular particles, the mass centers and mass momentums of represented particles are slightly different from that of real aggregates. Secondly, the quality of the images was not very good, which increased the difficulty to identify the boundary of individual particles. And because of this, some virtual particles might not keep their original shape accurately enough. Thirdly, the particle shapes are difficult to be accurately described using a small number of balls. Despite the discrepancy, it is worth noticing that the simulation based on real aggregate shapes did improve the agreement with the experimental observations.

Figure 16~Figure 18 present the contours of volumetric strains $\varepsilon_v$ at z=45~55mm by two simulations and by experiment, which have been projected in x-y plane. All of the three contours show strain dilation in the center part of the specimen while small strain contraction around the edge. The contours based on irregular particles have better agreement with the experimental observation, i.e. their contour shapes are closer to each other and have similar feature of strain localization. But the contours based on spherical particles are much different. Figure 19~Figure 21 present the contours of volumetric strains at y=45~55mm, which have been projected on x-z plane. In the experimental results, most of the strain contraction occurred at the top of the specimen and there was some strain dilation at the middle part. The simulation results based on
irregular particles had a similar trend with the experimental observations. But the contour based on spherical particles showed strain contraction almost in the entire specimen except certain regions, and the strain contraction was more significant than the experimental results.

The comparison between the simulated macro properties and the experimental results are presented in Table 7. For simulation on irregular particles, the vertical deformation of the entire specimen was 9.2 mm, close to experimental measurement, i.e. 9.8 mm. The relative difference is 5.8%, calculated as the percentage of ratio of absolute difference between two results to the experimental result. The simulated radial dilatancy of specimen (0.73 mm) is close to the experimental measurement (0.78 mm), with relative difference of 6.4%. The relative difference between the simulated global volumetric strain (-0.39) and the experimental measurements (-0.41) is 4.3%. As for the simulation on spherical particles, the vertical deformation of entire specimen is 12.3 mm, giving a relative difference of 25.5%; the radial dilation is 1.1 mm, giving a relative difference of 39.7%; and the global volumetric strain is -0.044, giving a relative difference of 6.6%. Though their global volumetric strains exhibit no big differences, the simulated global deformations based on spheres over estimated the specimen deformation and those based on real irregular particles are in good agreement with the experimental observations. The compatibility of simulated properties based on irregular particles with the experimental observations suggests that the DEM simulation incorporating real microstructure of material is a valid approach to predict the deformation of granular materials.

SUMMARY AND CONCLUSION

New methodologies for individual particle representation, particle kinematics and local strain quantification were developed for the analysis of a compression test using x-ray tomography imaging. These methodologies make it practical to simulate the micro-macro
behavior of granular materials in experiments whereby it is feasible to validate the continuum theory in true 3D and the quantitative accuracy of numerical simulation. The quantified particle translational displacements and local strains are reasonable.

Using clusters of balls to represent irregular particles, the material with actual microstructure was simulated by DEM approach. Comparing the simulation results based on spherical particles and those based on irregular particles, it’s found that particle shape has significant effect on both micro and macro properties of granular materials. At the micro level, it influences the contact interaction between particles. Thus the particle movements and micro strain field would be different for materials consisting of particles with different shape configuration. At the macro level, it affects the deformation and strength of material.

Most of the round particles had larger magnitude of translations. The material composed of round particles presented bigger vertical contraction and radial dilation in the simulation, which is not consistent with the experimental measurements. The simulated results based on real microstructure have better agreement with the experimental observations both at micro and macro level.

ACKNOWLEDGEMENT

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REFERENCES


Darve, F., Liquefaction phenomena of granular materials and constitutive stability, Engineering Computations (Swansea, Wales), v 13, n 7, p 5-28, 1996


Thornton, C. Applications of DEM to process engineering problems, Engineering Computations (Swansea, Wales), v 9, n 2, Apr, p 289-297, 1992


### Table 1: Properties of Materials, Specimen and Load

<table>
<thead>
<tr>
<th>Limestone Aggregates</th>
<th>Sponge</th>
<th>Container</th>
<th>Axial Load</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Size (mm)</strong></td>
<td><strong>Specific Gravity</strong></td>
<td><strong>Aggregate Number</strong></td>
<td><strong>Young’s modulus (Gpa)</strong></td>
</tr>
<tr>
<td>9.5~12.7</td>
<td>2.674</td>
<td>173</td>
<td>37</td>
</tr>
</tbody>
</table>

### Table 2: Example of Connection Status of Particle Cross-sections between Two Adjacent Slices

<table>
<thead>
<tr>
<th>Slice NO. = 70</th>
<th>Slice NO. = 71</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle cross-section i</td>
<td>$S_{\text{min}}$</td>
</tr>
<tr>
<td>1</td>
<td>0.31</td>
</tr>
<tr>
<td>2</td>
<td>0.37</td>
</tr>
<tr>
<td>3</td>
<td>0.21</td>
</tr>
<tr>
<td>4</td>
<td>0.57</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>26</td>
<td>-1</td>
</tr>
</tbody>
</table>

Note: This table shows that particle cross-section $i$ in slice 70 and $j$ in slice 71 belong to the same particle. $S_I$ is the minimum similarity index calculated between cross-section $i$ and $j$. If $S_{\text{min}}=-1$ & $j=0$, it means that particle disappears in slice No.71.

### Table 3: The Areas and Mass Centers of All Cross-sections of Particle No.50

<table>
<thead>
<tr>
<th>Particle No. = 50</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Slice No. (z)</strong></td>
</tr>
<tr>
<td>57</td>
</tr>
<tr>
<td>58</td>
</tr>
<tr>
<td>59</td>
</tr>
<tr>
<td>...</td>
</tr>
<tr>
<td>72</td>
</tr>
<tr>
<td>73</td>
</tr>
</tbody>
</table>

Note: This table presents cross-section $i$ in slice $z$ belonging to particle No.50 and its corresponding area and mass center coordinates.
Table 4: The Mass Center Coordinates and the Displacements for Individual Particles Obtained from Experimental Test

<table>
<thead>
<tr>
<th>Agg. No.</th>
<th>Coordinates of the Mass center (mm)</th>
<th>Displacement in x,y,z direction (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>x</td>
<td>y</td>
</tr>
<tr>
<td>1</td>
<td>46.15</td>
<td>29.55</td>
</tr>
<tr>
<td>2</td>
<td>56.19</td>
<td>34.22</td>
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<tr>
<td>3</td>
<td>39.01</td>
<td>33.28</td>
</tr>
<tr>
<td>4</td>
<td>29.51</td>
<td>37.41</td>
</tr>
<tr>
<td>5</td>
<td>65.51</td>
<td>37.97</td>
</tr>
<tr>
<td>6</td>
<td>50.78</td>
<td>47.22</td>
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<tr>
<td>7</td>
<td>72.69</td>
<td>47.58</td>
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<tr>
<td>8</td>
<td>30.07</td>
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<td>9</td>
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<td>50.11</td>
</tr>
<tr>
<td>10</td>
<td>61.13</td>
<td>52.16</td>
</tr>
</tbody>
</table>

Note: this table only presents calculated results of 10 particles.

Table 5: The Local Macro Strains and Macro Rotations from Experimental Test

<table>
<thead>
<tr>
<th>No.</th>
<th>$\varepsilon_x$</th>
<th>$\varepsilon_y$</th>
<th>$\varepsilon_z$</th>
<th>$\varepsilon_{xy}$</th>
<th>$\varepsilon_{yz}$</th>
<th>$\varepsilon_{xz}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.00</td>
<td>-0.05</td>
<td>-0.05</td>
<td>-0.04</td>
<td>0.02</td>
<td>-0.04</td>
</tr>
<tr>
<td>2</td>
<td>0.70</td>
<td>-1.10</td>
<td>-0.80</td>
<td>-0.43</td>
<td>-0.08</td>
<td>-0.97</td>
</tr>
<tr>
<td>3</td>
<td>0.07</td>
<td>-0.08</td>
<td>0.00</td>
<td>0.10</td>
<td>0.11</td>
<td>0.30</td>
</tr>
<tr>
<td>4</td>
<td>-0.14</td>
<td>0.03</td>
<td>3.35</td>
<td>0.15</td>
<td>0.33</td>
<td>-0.42</td>
</tr>
<tr>
<td>5</td>
<td>0.17</td>
<td>-0.26</td>
<td>-0.04</td>
<td>0.10</td>
<td>0.05</td>
<td>-0.09</td>
</tr>
<tr>
<td>6</td>
<td>0.02</td>
<td>0.12</td>
<td>-0.21</td>
<td>0.05</td>
<td>0.09</td>
<td>-0.05</td>
</tr>
<tr>
<td>7</td>
<td>0.01</td>
<td>0.03</td>
<td>-0.09</td>
<td>-0.01</td>
<td>0.05</td>
<td>-0.04</td>
</tr>
<tr>
<td>8</td>
<td>0.20</td>
<td>0.07</td>
<td>0.02</td>
<td>0.00</td>
<td>0.14</td>
<td>-0.03</td>
</tr>
<tr>
<td>9</td>
<td>-0.04</td>
<td>0.07</td>
<td>0.45</td>
<td>-0.04</td>
<td>0.03</td>
<td>-0.16</td>
</tr>
<tr>
<td>10</td>
<td>2.32</td>
<td>-1.03</td>
<td>-0.14</td>
<td>-2.11</td>
<td>-1.19</td>
<td>2.58</td>
</tr>
</tbody>
</table>

Note: this table only presents calculated results of 10 particles.
Table 6: Comparison of Coordination Number between DEM Simulation and Experiment Measurements

<table>
<thead>
<tr>
<th>Results</th>
<th>Experiments</th>
<th>DEM-Sphere</th>
<th>DEM-Irr. Particle</th>
</tr>
</thead>
<tbody>
<tr>
<td>coordination number(before test)</td>
<td>4.930</td>
<td>3.030</td>
<td>4.930</td>
</tr>
<tr>
<td>coordination number(after test)</td>
<td>6.130</td>
<td>6.710</td>
<td>6.650</td>
</tr>
<tr>
<td>change</td>
<td>1.200</td>
<td>3.680</td>
<td>1.720</td>
</tr>
</tbody>
</table>

Table 7: Comparison of Macro Properties between DEM Simulation and Experimental Measurements

<table>
<thead>
<tr>
<th>Results</th>
<th>Experiment Irregular Particle</th>
<th>DEM Irregular Particle</th>
<th>%Relative Diff.</th>
<th>DEM Sphere</th>
<th>%Relative Diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertical contraction(mm)</td>
<td>9.800</td>
<td>9.230</td>
<td>5.816</td>
<td>12.300</td>
<td>25.510</td>
</tr>
<tr>
<td>Radial dilation(mm)</td>
<td>0.780</td>
<td>0.730</td>
<td>6.410</td>
<td>1.090</td>
<td>39.744</td>
</tr>
<tr>
<td>Global Volume Strain</td>
<td>-0.041</td>
<td>-0.039</td>
<td>4.368</td>
<td>-0.044</td>
<td>6.652</td>
</tr>
<tr>
<td>change of porosity</td>
<td>0.024</td>
<td>0.023</td>
<td>5.859</td>
<td>0.027</td>
<td>13.858</td>
</tr>
</tbody>
</table>
Slice $j$  \hspace{1cm} Slice $j+1$

New Particle Emerge

Figure 1: Illustration of New Particle Emerging in the next slice

Slice $j$  \hspace{1cm} Slice $j+1$

This Particle Disappear In Next Slice

Figure 2: Illustration of Exist Particle Disappearing in the Next Slice

Slice $j$  \hspace{1cm} Slice $j+1$

This Particle Disappear in the Next Slice

New Particle Emerge at the Similar Location

Figure 3: Illustration of Exist Particle Disappearing and New Particle Emerging at the similar location
Input $X_{z,i}$, $Y_{z,i}$, $Z_{z,i}$, Area $z_i$, $S_{I0}$

$$S_{I_{z,i}} = |X_{z+1,j} - X_{z,i}| + |Y_{z+1,j} - Y_{z,i}|$$

For particle $PC_{z,j}$ find $PC_{z+1,j}$ giving minimum $S_{I_{z,i}}$

$$S_{I_{min}} = S_{I_{z,i}} \ ; \ P_{next_{z,i}} = PC_{z+1,j}$$

If more than one particle in the $z$ slide are corresponded to the same particle in the $z+1$ slide

Smallest $S_{I_{min}}$ ?

$P_{next_{z,i}} = 0, S_{I_{min}} = -1$

$S_{I_{min}} > S_{I0}$ ?

Number of slides that particle $P_k$ occupies; and Cross section code, mass center, Area for $P_k$ in each slide.

Figure 4: Flow Chart to Identify Individual Particles.
(The Input Parameters are obtained from imaging analysis.)
Input $X_{z,i}$, $Y_{z,i}$, $Z_{z,i}$, Area $z_i$, $P_{z,i}$, $H_{z,i}$

$V_k = \sum \left( \left( \text{Area}_{z_{k,j}} + \text{Area}_{z_{k,i}} \right) H_{z_{k,j}}/2 \right)$

$X_{c_k} = \frac{1}{V_k} \sum \left( \left( \text{Area}_{z_{k,i}} + \text{Area}_{z_{k,j}} \right) H_{z_{k,i}} (X_{z_{k,i}} + X_{z_{k,j}})/4 \right)$

$Y_{c_k} = \frac{1}{V_k} \sum \left( \left( \text{Area}_{z_{k,i}} + \text{Area}_{z_{k,j}} \right) H_{z_{k,i}} (Y_{z_{k,i}} + Y_{z_{k,j}})/4 \right)$

$Z_{c_k} = \frac{1}{V_k} \sum \left( \left( \text{Area}_{z_{k,i}} + \text{Area}_{z_{k,j}} \right) H_{z_{k,i}} (Z_{z_{k,i}} + Z_{z_{k,j}})/4 \right)$

$SI_p = \left| X_{c_{p}}^{b} - X_{c_{p}}^{a} \right| + \left| Y_{c_{p}}^{b} - Y_{c_{p}}^{a} \right| + \left| Z_{c_{p}}^{b} - (Z_{c_{p}}^{a} + \Delta t / h * Z_{c_{p}}^{a}) \right|$

Pair of particles giving the minimum $SI_p$?

If two $P_k^a$ points to the same original particle

Smaller $SI = \left| V_k^{b} - V_k^{a} \right|$?

Particle $P_k^a$ (after test) corresponding to original particle $P_k^b$
Displacements of particle $P_k$ in x, y, z direction after test.

Figure 5: Flow Chart to Recognize Particles after the Test
(The input parameters are obtained from image analysis and results of particle detection)
Figure 6: Illustration of 3D Movements of 4 Adjacent Particles in Compression Test
Figure 7: $\varepsilon_x$ Contour in XY Plane-Experimental Result

Figure 8: $\varepsilon_z$ Contour in XZ Plane-Experimental Results
(Vertical line is drawn to help read the strain value every 10mm at z direction)
Figure 9: Microstructure of Specimen Composed of Irregular Particles
(Irregular particles are represented by clusters of balls)

Figure 10: Microstructure of Specimen Composed of Spherical Particles
Figure 11: Illustration of Particle Translational Movements-Experimental Results

Figure 12: Illustration of Particle Translational Movements-Simulation on Irregular Particles

Figure 13: Illustration of Particle Translational Movements-Simulation on Spherical Particles
Figure 14: Simulated Magnitudes of Spherical Particle Translations V.S. Experimental Measurements

Figure 15: Simulated Magnitudes of Irregular Particle Translations V.S. Experimental Measurements
Figure 16: $\varepsilon_v$ Contour in XY Plane (Experimental Results)

Figure 17: $\varepsilon_v$ Contour in XY Plane (Simulations on Irregular Particles)

Figure 18: $\varepsilon_v$ Contour in XY Plane (Simulations on Spherical Particles)
Figure 19: $\varepsilon_v$ Contour in XZ Plane (Experimental Results)

Figure 20: $\varepsilon_v$ Contour in XZ Plane (Simulations on Irregular Particles)

Figure 21: $\varepsilon_v$ Contour in XZ Plane (Simulation on Spherical Particles)